Computational Aspects in the Simulation of Rarefied Gas Flows

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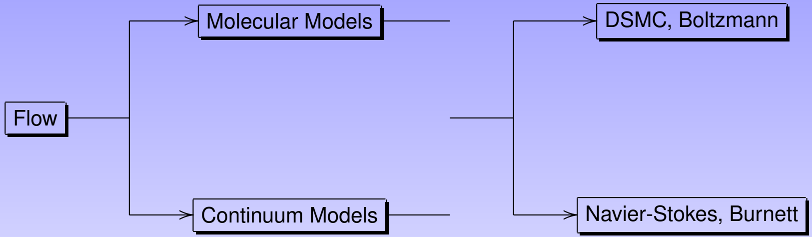
Gas Flows x Knudsen number (λ /a)

- hydrodynamic regime ($Kn < 0,01$): NS equations
- "slip flow" - moderate gas rarefaction ($0,01 < Kn < 0,1$): NS + velocity slip (temperature jump) boundary conditions
- transition regime ($0,1 < Kn < 10$): Boltzmann equation
- free-molecular regime :analytical solutions

Modeling


Flow
Molecular Models
Continuum Models
DSMC, Boltzmann
Navier-Stokes, Burnett

RGD and Applications

- Aerospace Sciences
- Recently: MEMS and NEMS

Motivation: RGD x recent applications

MEMS

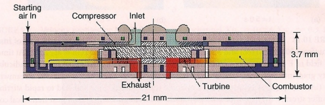
(Micro) Eletro-Mechanical Systems: devices with charactheristic length $1\mu m < L < 1mm$ *which combines eletrical and mechanical components (size + cost)*

- Computers (design of comp. - 50nm) and printers (pumps)
- acelerometers for airbags (lower size and cost)
- micro mirrors for high optical definition
- Medical Equip: pressure sensors for catheters, drug delivery
- Clinical exams

MEMS

Flow Physics: Surface effects and other physical (nonfamiliar) effects

Microengine



COLOR FIGURE 11.6 Schematic of the MIT Microengine, showing the air path through the compressor, combustor, and turbine. Forward and aft thrust bearings located on the centerline hold the rotor in axial equilibrium, while a journal bearing around the rotor periphery holds the rotor in radial equilibrium.

Source: MEMS Handbook, Gad El Hak

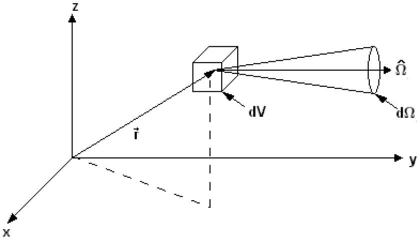
Deterministic Approach

- The Boltzmann Equation
- Other applications: Remote Sensing, Nuclear Engineering, Radiotherapy

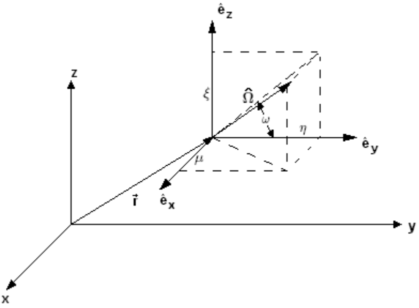
Research in Brasil: different approaches

- Garcia, R. D. M. (IEAv-CTA)
- Kraemer, G (UFPR)
- Santos, W. (INPE)
- Sharipov, F. (UFPR)

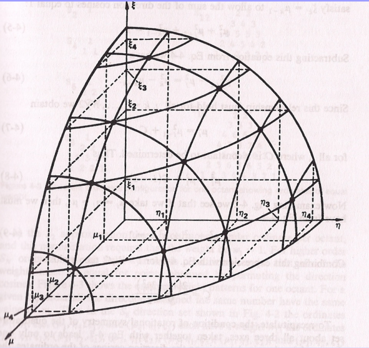
Geometry



Geometry



Discrete Ordinates



Reference: Lewis and Miller Jr., 1993.

LBE - rigid spheres

the non-linear Boltzmann

$$\mathbf{v} \cdot \nabla_r f(\mathbf{r}, \mathbf{v}) = J(f', f) \qquad (1)$$

$f(\mathbf{r}, \mathbf{v})$ is the gas atom space and velocity distribution function; (f' and f are associated with, respectively, before and after collisions distributions); J is the collision operator.

$$f(\mathbf{r}, \mathbf{v}) = f_0(\mathbf{v})[1 + h(\mathbf{r}, \mathbf{v})] \qquad (2)$$

h is a perturbation to the absolute Maxwellian $f_0(\mathbf{v})$; k is the Boltzmann constant, T_0 is a reference temperature, m_0 is the mass and n_0 is the equilibrium density of the gas.

$$\mathbf{c} = \mathbf{v}(m/2kT_0)^{1/2}, \qquad (4)$$

LBE - rigid spheres

Linearized Boltzmann Equation (LBE)

$$c_x \frac{\partial}{\partial \tau} h(\tau, \mathbf{c}) + \varepsilon h(\tau, \mathbf{c}) =$$
$$\varepsilon \pi^{-3/2} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} e^{-c'^2} h(\tau, \mathbf{c}') F(\mathbf{c}' : \mathbf{c}) dc'_x dc'_y dc'_z, \quad (5)$$

dimensionless variable $\tau = x/l$, arbitrary mean-free path l,

$$\varepsilon = \sigma_0^2 n_0 \pi^{1/2} l, \quad (6)$$

σ_0 is the collision diameter of the gas particles (in the rigid-sphere approximation).

Kernel

Rigid Spheres

$$F(\mathbf{c}' : \mathbf{c}) = \frac{1}{2\pi} \sum_{n=0}^{\infty} \sum_{m=0}^{N} (\frac{2n+1}{2})(2 - \delta_{0,m}) P_n^m(\mu') P_n^m(\mu) \times f_n(c', c) \cos m(\phi' - \phi)$$

The temperature-jump problem (half-space)

Boundary Conditions

$$h(0, c_x, c_y, c_z) = (1-\alpha)h(0, -c_x, c_y, c_z) + \frac{2\alpha}{\pi}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{0}^{\infty} e^{-c'^2} h(0, -c'_x, c'_y, c'_z) c'_x dc'_x dc'_y dc'_z, \quad (18)$$

for $c_x > 0$

$$\lim_{\tau\to\infty} \frac{d}{d\tau} T(\tau) = \mathcal{K}, \quad (19)$$

where $\mathcal{K}$ is constant.

$\alpha \in (0, 1]$ is the accommodation coefficient (Maxwell law) .

Quantities of Interest

In terms of the perturbation distribution h

- perturbation of density

$$N(\tau) = \pi^{-3/2} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \mathrm{e}^{-c^2} h(\tau, \mathbf{c}) \mathrm{d}c_x \mathrm{d}c_y \mathrm{d}c_z, \quad (13)$$

- perturbation of temperature

$$T(\tau) = \frac{2}{3} \pi^{-3/2} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \mathrm{e}^{-c^2} \left(c^2 - 3/2 \right) \times h(\tau, \mathbf{c}) \mathrm{d}c_x \mathrm{d}c_y \mathrm{d}c_z \quad (14)$$

Challenges

- *Multidimensional Geometries*
- *Accuracy, Computational Time*

In this talk

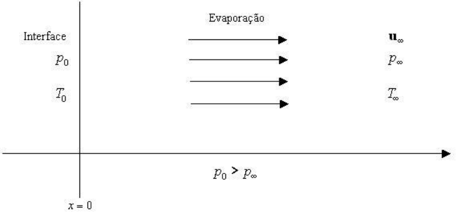
- Our work: Spectral (Analytical) Methods, Accuracy, Computational Time
- Analytical $\times$ Computational Aspects

Main Computational Steps

- Main basic problem: several times (inverse problems, azimuthal dependence, multidimensional)
- Definition of a Quadrature Scheme for the Integral Term
- Eigenvalue System
- Linear System

- *Kinetic Models*
- *Discrete Ordinates Version* $\times$ *Order of the System*
- *Closed Form Solutions: Post Processing Results*
- *Nonlinear Aspects*

Strong Evaporation Problem



Steady-state limit of the following (Ytrehus, 1976): • a liquid (or solid) is initially in equilibrium with its pure vapor which occupies the half-space $x \geq 0$ at uniform temperature and pressure T_0 and p_0, respectively.

• At time $t = 0$ the pressure level in the vapor changes discontinuously to the value p_∞ and it is kept at this value.

• Evaporation (condensation) begins, through the phase boundary, according to whether the pressure level p_∞ is below (above) the saturation pressure p_0.

• Far from the phase boundary – uniform equilibrium flow with constant parameters ϱ_∞, v_∞ and T_∞

• Half-space problem $\times$ Knudsen layer

Definitions

The density $\varrho(x)$, mass velocity $v(x)$ and temperature $T(x)$ in Eq. (2), are defined as

$$\varrho(x) = \int_{-\infty}^{\infty} f(x,\xi)\mathrm{d}\xi, \tag{3}$$

$$\varrho(x)v(x) = \int_{-\infty}^{\infty} \xi f(x,\xi)\mathrm{d}\xi \tag{4}$$

$$\varrho(x)RT(x) = \int_{-\infty}^{\infty} [\xi - v(x)]^2 f(x,\xi)\mathrm{d}\xi. \tag{5}$$

we assume that far downstream the gas relaxes to an equilibrium distribution characterized by steady drift velocity v_∞, density ϱ_∞ and temperature T_∞,

$$f_\infty(\xi) = \lim_{x\to\infty} \phi(x,\xi) = \frac{\varrho_\infty}{\sqrt{2\pi RT_\infty}} \exp\left\{-\frac{(\xi - v_\infty)^2}{2RT_\infty}\right\}. \tag{6}$$

Linearization

we linearize $f(x, \xi)$ and $\phi(x, \xi)$ around $f_\infty(\xi)$ (absolute Maxwellian)

$$f(x, \xi) = f_\infty(\xi)[1 + h(x, \xi)], \tag{7}$$

to obtain the one-dimensional linearized equation written in terms of the perturbation function h.

$$\tau = \eta x(2RT_\infty)^{-1/2},\ c = \xi(2RT_\infty)^{-1/2},\ u = v_\infty(2RT_\infty)^{-1/2},$$

are the dimensionless variables. We note that u is the normalized downstream drift velocity.

Linearized Model Equation

$$c\frac{\partial}{\partial\tau}h(\tau,c)+h(\tau,c)=\pi^{-1/2}\int_{-\infty}^{\infty}e^{-(c'-u)^2}K(c',c:u)h(\tau,c')dc', \tag{8}$$

where

$$K(c',c:u)=1+2(c'-u)(c-u)+2\{(c'-u)^2-1/2\}\{(c-u)^2-1/2\}, \tag{9}$$

is the scattering kernel.

OBS

$$(c+u)\frac{\partial}{\partial\tau}h=Lh$$

Boundary Conditions

$x = 0$ in Eq. (7), to find (for $\xi > 0$)

$$h(0,\xi) = \frac{f(0,\xi) - f_\infty(\xi)}{f_\infty(\xi)}, \tag{11}$$

where $f(0,\xi)$ is the Maxwellian distribution, given by Eq. (2), evaluated at $x = 0$

$$f(0,\xi) = \frac{\varrho_0}{\sqrt{2\pi R T_0}} \exp\left\{ -\frac{(\xi - v_0)^2}{2RT_0} \right\}. \tag{12}$$

We then linearize $f(0,\xi)$ around $f_\infty(\xi)$ to obtain the dimensionless boundary condition (for $c > 0$)

$$h(0,c) = \Delta\varrho_0 + 2(c-u)(u_0-u) + \left[(c-u)^2 - 1/2\right]\Delta T_0, \tag{13}$$

$$u_0 = v_0(2RT_\infty)^{-1/2}, \qquad \Delta\varrho_0 = \frac{\varrho_0 - \rho_\infty}{\varrho_\infty} \qquad \textit{and} \qquad \Delta T_0 = \frac{T_0 - T_\infty}{T_\infty}. \quad \text{(14 a, b, c)}$$

On the other hand, when $x \to \infty$, $f(x,\xi)$ approaches $f_\infty(\xi)$ and, looking back Eq. (7), we then find the condition

$$\lim_{\tau\to\infty} h(\tau, c) = 0. \tag{15}$$

Quantities of Interest

In terms of the perturbation distribution h

- density perturbation

$$\Delta\varrho(\tau) = \pi^{-1/2} \int_{-\infty}^{\infty} \mathrm{e}^{-(c-u)^2} h(\tau, c)\mathrm{d}c, \qquad (16)$$

- velocity perturbation

$$\Delta v(\tau) = \frac{\pi^{-1/2}}{u} \int_{-\infty}^{\infty} \mathrm{e}^{-(c-u)^2} (c-u) h(\tau, c)\mathrm{d}c \qquad (17)$$

- temperature perturbation

$$\Delta T(\tau) = \pi^{-1/2} \int_{-\infty}^{\infty} \mathrm{e}^{-(c-u)^2} [2(c-u)^2 - 1] h(\tau, c)\mathrm{d}c. \qquad (18)$$

A Reformulation

$$G(\tau, c) = \mathrm{e}^{-(c-u)^2} h(\tau, c) \tag{19}$$

G Problem

$$c\frac{\partial}{\partial \tau} G(\tau, c) + G(\tau, c) = \pi^{-1/2} e^{-(c-u)^2} \int_{-\infty}^{\infty} K(c', c : u) G(\tau, c') dc', \tag{20}$$

Boundary Conditions

$$G(0, c) = \left\{ \Delta \varrho_0 + 2(c-u)(u_0 - u) + \left[(c-u)^2 - 1/2 \right] \Delta T_0 \right\} e^{-(c-u)^2}, \; c > 0 \tag{21}$$

$$\lim_{\tau \to \infty} G(\tau, c) = 0. \tag{22}$$

New definitions for Density, Temperature and Velocity Perturbations

A Discrete Ordinates Solution

$$G(\tau, c) = \Phi(\nu, c)e^{-\tau/\nu}. \tag{26}$$

If we substitute Eq. (26) into Eq. (20) we obtain

$$(1 - c/\nu)\Phi(\nu, c) = \pi^{-1/2}e^{-(c-u)^2} \int_{-\infty}^{\infty} K(c', c : u)\Phi(\nu, c')dc'. \tag{27}$$

normalization conditions: we integrate Eq. (27), over all c, to find

$$\int_{-\infty}^{\infty} c\Phi(\nu, c)dc = 0. \tag{28}$$

we can multiply Eq. (27) by $(c - u)$ and integrate the resultant equation over all c to find

$$\int_{-\infty}^{\infty} c^2\Phi(\nu, c)dc = 0. \tag{29}$$

we rewrite Eq. (27), as

$$(1 - c/\nu)\Phi(\nu, c) = \pi^{-1/2}e^{-(c-u)^2} Q(c : u) \int_{-\infty}^{\infty} \Phi(\nu, c')dc', \tag{30}$$

with

$$Q(c : u) = 1 + 2u^2 + 2(c^2 + u^2 - 1/2)(u^2 - 1/2) - 4cu^3. \tag{31}$$

we note that the exponential term, in Eq. (30)can be expressed as

$$e^{-(c-u)^2} = e^{-(c^2+u^2)}[\text{senh}(2cu) + \cosh(2cu)] \tag{32}$$

$$(1 - c/\nu)\Phi(\nu, c) = \psi(c:u)[A(c:u) + B(c:u)] \int_{-\infty}^{\infty} \Phi(\nu, c')\mathrm{d}c', \tag{33}$$

where

$$\psi(c:u) = \pi^{-1/2}\mathrm{e}^{-(c^2+u^2)}, \tag{34}$$

$$A(c:u) = [1 + 2u^2 + 2(c^2 + u^2 - 1/2)(u^2 - 1/2)]\cosh(2cu) - 4cu^3\mathrm{senh}(2cu) \tag{35}$$

and

$$B(c:u) = [1 + 2u^2 + 2(c^2 + u^2 - 1/2)(u^2 - 1/2)]\mathrm{senh}(2cu) - 4cu^3\cosh(2cu). \tag{36}$$

$$(1 - c/\nu)\Phi(\nu, c) = \psi(c : u)[A(c : u) + B(c : u)] \int_0^\infty [\Phi(\nu, c') + \Phi(\nu, -c')] \mathrm{d}c'. \quad (37)$$

Then we introduce a (**half-range**) quadrature scheme $[0, \infty)$, to approximate the integral term of the above equation, such that

$$(1 - c/\nu)\Phi(\nu, c) = \psi(c : u)[A(c : u) + B(c : u)] \sum_{k=1}^{N} w_k [\Phi(\nu, c_k) + \Phi(\nu, -c_k)]. \quad (38)$$

Here c_k and w_k are, respectively, the N nodes and weights of the (arbitrary) quadrature scheme. If we now evaluate Eq. (38) in $c = \pm c_i$, for $i = 1, \dots, N$, and note that $\psi(c : u)$ and $A(c : u)$ are even functions,

$$\psi(c : u) = \psi(-c : u), \qquad A(c : u) = A(-c : u), \qquad (39\text{ a, b})$$

and $B(c : u)$ is an odd function,

$$B(c : u) = -B(-c : u), \quad (40)$$

we obtain the discrete-ordinates version of the Eq. (37) as

$$(1 \mp c_i/\nu)\Phi(\nu, \pm c_i) = \psi(c_i : u)[A(c_i : u) \pm B(c_i : u)] \sum_{k=1}^{N} w_k [\Phi(\nu, c_k) + \Phi(\nu, -c_k)]. \quad (41)$$

Matrix Form

We express now Eq. (41) in a matrix form, as

$$(\mathbf{I} - \mathbf{M}/\nu)\,\boldsymbol{\Phi}_+(\nu) = \boldsymbol{\Psi}[\mathbf{A} + \mathbf{B}]\mathbf{W}\boldsymbol{\Phi}_+(\nu) + \boldsymbol{\Phi}_-(\nu)] \tag{42}$$

and

$$(\mathbf{I} + \mathbf{M}/\nu)\,\boldsymbol{\Phi}_-(\nu) = \boldsymbol{\Psi}[\mathbf{A} - \mathbf{B}]\mathbf{W}[\boldsymbol{\Phi}_+(\nu) + \boldsymbol{\Phi}_-(\nu)], \tag{43}$$

where $\mathbf{I}$ is the $N \times N$ identity matrix, $\mathbf{M}$, $\boldsymbol{\Psi}$, $\mathbf{A}$, $\mathbf{B}$ and $\mathbf{W}$ are $N \times N$ matrices defined by

$$\mathbf{M} = \text{diag}\,\{c_1, \ldots, c_N\}\,, \tag{44}$$

$$\boldsymbol{\Psi} = \text{diag}\,\{\psi(c_1 : u), \ldots, \psi(c_N : u)\}\,, \tag{45}$$

$$\mathbf{A} = \text{diag}\,\{A(c_1 : u), \ldots, A(c_N : u)\}\,, \tag{46}$$

$$\mathbf{B} = \text{diag}\,\{B(c_1 : u), \ldots, B(c_N : u)\} \tag{47}$$

and

$$\mathbf{W}_{ij} = [w_j], \tag{48}$$

for $i, j = 1, \ldots, N$.

Eigenvalue Problem

Continuing, here, $\mathbf{\Phi}_{\pm}(\nu)$ are $N \times 1$ vectors, such that

$$\mathbf{\Phi}_{\pm}(\nu) = \left[\begin{array}{ccc} \Phi(\nu, \pm c_1) & \cdots & \Phi(\nu, \pm c_N) \end{array} \right]^T, \tag{49}$$

where T denote the transpose operation.
e now add and subtract Eqs. (42) and (43) to find the equations

$$\mathbf{U} - \frac{1}{\nu}\mathbf{MV} = 2\mathbf{\Psi AWU} \quad \text{and} \quad \mathbf{V} - \frac{1}{\nu}\mathbf{MU} = 2\mathbf{\Psi BWU}, \tag{50 a, b}$$

with

$$\mathbf{U} = \mathbf{\Phi}_{+}(\nu) + \mathbf{\Phi}_{-}(\nu) \quad \text{and} \quad \mathbf{V} = \mathbf{\Phi}_{+}(\nu) - \mathbf{\Phi}_{-}(\nu). \tag{51 a, b}$$

$\mathbf{\Phi}_{+}(\nu)$ and $\mathbf{\Phi}_{-}(\nu)$ are the vectors defined in Eq. (49). Substituting Eq. (50b) into Eq. (50a) we find a quadratic eigenvalue problem

$$[\mathbf{I}\lambda^2 + 2\mathbf{M}^{-1}\mathbf{\Psi BW}\lambda + 2\mathbf{M}^{-2}\mathbf{\Psi AW} - \mathbf{M}^{-2}]\mathbf{U} = \mathbf{0}, \tag{52}$$

where the eigenvalues are given by

$\lambda = \nu^{-1}$

Quadratic Eigenvalue Problem

Standard eigenvalue problem

$$\begin{bmatrix} \mathbf{0} & \mathbf{I} \\ -\mathbf{G} & -\mathbf{F} \end{bmatrix} \begin{bmatrix} \mathbf{U} \\ \lambda\mathbf{U} \end{bmatrix} = \lambda \begin{bmatrix} \mathbf{U} \\ \lambda\mathbf{U} \end{bmatrix}, \tag{53}$$

where

$$\mathbf{F} = 2\mathbf{M}^{-1}\boldsymbol{\Psi}\mathbf{B}\mathbf{W} \quad \text{and} \quad \mathbf{G} = 2\mathbf{M}^{-2}\boldsymbol{\Psi}\mathbf{A}\mathbf{W} - \mathbf{M}^{-2}. \tag{54 a, b}$$

• Conservative problem:
the number of degenerate eigenvalues depends on the value of u (the downstream drift velocity)

- for $u = 0$, we find four degenerated eigenvalues, $N - 2$ positive and too $N - 2$ negative eigenvalues;
- for $u^2 < 3/2$, we find three degenerated eigenvalues, $N - 2$ positive and $N - 1$ negative eigenvalues;
- for $u^2 = 3/2$, we find four degenerated eigenvalues, $N - 3$ positive and $N - 1$ negative eigenvalues;
- for $u^2 > 3/2$, we find three degenerated eigenvalues, $N - 3$ positive and N negative eigenvalues.

General Solution

general discrete ordinates solution of Eq. (20) in the form

$$G(\tau, \pm c_i) = A_1^* G_1(\pm c_i) + A_2^* G_2(\pm c_i) + A_3^* G_3(\pm c_i) + A_4^* G_4(\tau, \pm c_i) + \sum_{j=1}^{2N-4} A_j \Phi(\nu_j, \pm c_i) e^{-\tau/\nu_j} \tag{58}$$

for $u = 0$ and $u^2 = 3/2$, and

$$G(\tau, \pm c_i) = A_1^* G_1(\pm c_i) + A_2^* G_2(\pm c_i) + A_3^* G_3(\pm c_i) + \sum_{j=1}^{2N-3} A_j \Phi(\nu_j, \pm c_i) e^{-\tau/\nu_j} \tag{59}$$

for $0 < u^2 < 3/2$ and $u^2 > 3/2$, where the introduced exact solutions are given by

$$G_1(c) = e^{-(c-u)^2}, \qquad G_2(c) = (c-u)e^{-(c-u)^2}, \qquad G_3(c) = (c-u)^2 e^{-(c-u)^2} \tag{60 a, b, c}$$

and (only for $u = 0$ and $u^2 = 3/2$)

$$G_4(\tau, c) = (\tau - c) Q(c : u) e^{-(c-u)^2}. \tag{61}$$

the next step is to determine the arbitrary constants present in the solution (Eq. (58) or (59)). We use the boundary conditions for doing that. We then substitute the general solution, Eqs. (58) and (59), into Eq. (22) to obtain, for $u^2 < 3/2$,

$$G(\tau, \pm c_i) = \sum_{j=1}^{N-2} A_j \Phi(\nu_j, \pm c_i) e^{-\tau/\nu_j} \tag{62}$$

and for $u^2 \geq 3/2$

$$G(\tau, \pm c_i) = \sum_{j=1}^{N-3} A_j \Phi(\nu_j, \pm c_i) \mathrm{e}^{-\tau/\nu_j}, \tag{63}$$

where, here, ν_j are the positive separations constants. In addition, the discrete-ordinates version of the interface boundary condition, Eq. (21), is

$$G(0, c_i) = \left\{ \Delta\varrho_0 + 2(c_i - u)(u_0 - u) + \left[(c_i - u)^2 - 1/2 \right] \Delta T_0 \right\} \mathrm{e}^{-(c_i - u)^2}, \tag{64}$$

for $i = 1, \ldots, N$.

In this way, if we substitute Eq. (62) into Eq. (64), we obtain for $u^2 < 3/2$ the square linear system $N \times N$

$$\sum_{j=1}^{N-2} A_j \Phi(\nu_j, c_i) - \Delta\varrho_0 e^{-(c_i-u)^2} - [(c_i-u)^2 - 1/2]\Delta T_0 e^{-(c_i-u)^2} = 2(c_i-u)(u_0-u)e^{-(c_i-u)^2}, \quad (65)$$

for $i = 1, \ldots, N$.

If we substitute Eq. (63) into Eq. (64), we obtain for $u^2 \geq 3/2$ the rectangular linear system $N \times N - 1$

$$\sum_{j=1}^{N-3} A_j \Phi(\nu_j, c_i) - \Delta\varrho_0 e^{-(c_i-u)^2} - [(c_i-u)^2 - 1/2]\Delta T_0 e^{-(c_i-u)^2} = 2(c_i-u)(u_0-u)e^{-(c_i-u)^2}, \quad (66)$$

for $i = 1, \ldots, N$.

- Existence condition
- Once we solve Eqs. (65) we find the coefficients A_j and the quantities $\Delta\varrho_0$ and ΔT_0 defined in Eqs. (14b) and (14c).

Quantities of Interest

Thus, we substitute Eq. (62) into Eqs. (23) to (25) and we use the normalization conditions given by Eqs. (28) and (29) to express the final form of the density perturbation

$$\Delta\varrho(\tau) = \pi^{-1/2} \sum_{j=1}^{N-2} A_j e^{-\tau/\nu_j} \sum_{k=1}^{N} w_k [\Phi(\nu_j, c_k) + \Phi(\nu_j, -c_k)], \quad (67)$$

velocity and temperature perturbations, respectively,

$$\Delta v(\tau) = -\Delta\varrho(\tau) \quad \text{and} \quad \Delta T(\tau) = (2u^2 - 1)\Delta\varrho(\tau). \quad (68\text{ a, b})$$

Nonlinear Aspects

BGK model

$$\xi \frac{\partial}{\partial x} f(x, \xi) = \eta[\phi(x, \xi) - f(x, \xi)], \tag{1}$$

where $f(x, \xi)$ is the distribution function, ξ is the molecular velocity in the x direction, η is an appropriate collision frequency, $\phi(x, \xi)$ is a local Maxwell distribution,

$$\phi(x, \xi) = \frac{\varrho(x)}{\sqrt{2\pi RT(x)}} \exp\left\{-\frac{[\xi - v(x)]^2}{2RT(x)}\right\}, \tag{2}$$

and R is the specific gas constant.

PP procedure

- “post-processing (PP)” procedure. we consider the proposed nonlinear model, given by Eq. (1) to(5), with boundary conditions defined in Eqs. (6) and (12), rewritten in terms of the dimensionless variables given in Eqs. (10).
- We then use the quantities evaluated by the ADO method, Eqs. (67) and (68), into Eq. (2), which defines the Maxwellian distribution.
- Continuing, we substitute this distribution in the right-hand side of Eq. (1), which is then solved for a known distribution $\phi(x, \xi)$.
- The solution defines the original f distribution, which is then used to evaluated again Eqs. (3) to (5) – the macroscopic quantities for the gas.

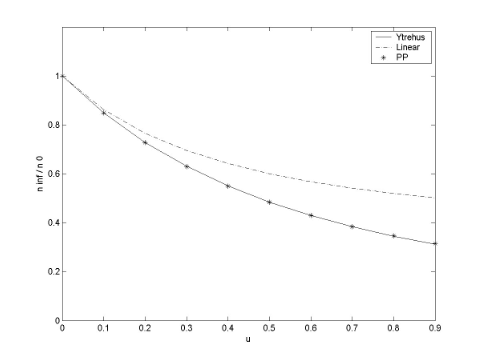
Computational Procedures

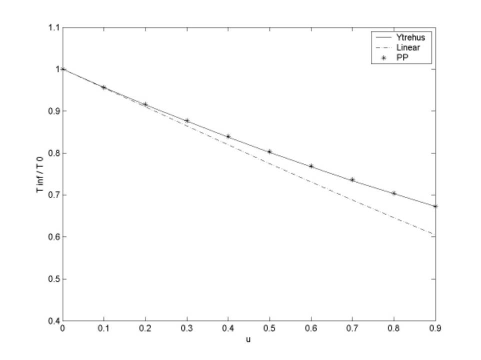
- first step is to define the quadrature scheme (N quadrature points c_k and the weights w_k)
- the solution of an eigenvalue problem, Eq. (53), to obtain the separation constants ν_j and the elementary solutions $\mathbf{\Phi}_{\pm}(\nu_j)$;
- the solution of a linear system, given by Eq. (65);
- the evaluation of the density, velocity and temperature perturbations, Eqs. (67) and (68). Still, from the solution of Eq. (65) we are able to get the quantities $\Delta\varrho_0$ and ΔT_0, Eqs. (14b) and (14c).
- The quantities listed above are then used, in what we called "post-processing" procedure, in Eqs. (1) to (5).
- New definitions for quadrature schemes

Numerical Results

- FORTRAN program, using, in general, $N = 80$ quadrature points.
- The computational time required for generating all quantities of interest for one value of u is less than one second in a Pentium IV (2.66GHz, 1.5GB RAM).
- If we increase N up to $N = 200$, all digits listed in the tables are preserved (plus or minus one in the last digit): 6-7 (L) and 5 (PP).
- Checking with results available in the literature, for the linearized problem, for ϱ_∞/ϱ_0 and T_∞/T_0. We obtained agreement with all digits (4) listed in that reference.

Ratios




Ytrehus
Linear
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T inf / T 0
u
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1
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0.4
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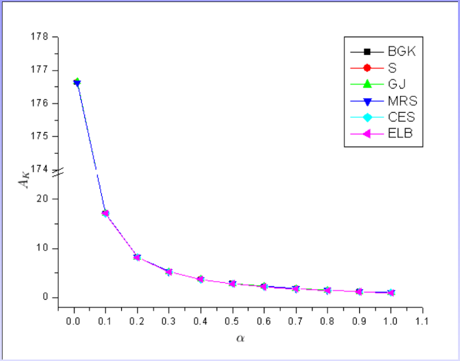
0.9

In general

- Strong Evaporation Problem: Profiles $\times$ Ratios
- Unified solutions for kinetic model equations: concise, accurate and fast


178
177
176
175
174
20
10
0
A_K
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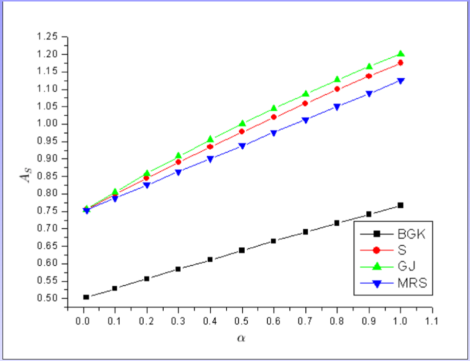
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1.0
1.1
α
BGK
S
GJ
MRS
CES
ELB

General analysis



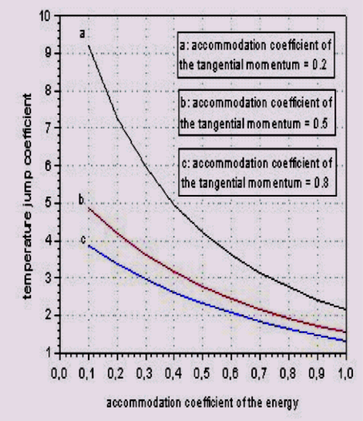


Figure 2: Temperature jump coefficient, $N = 40$

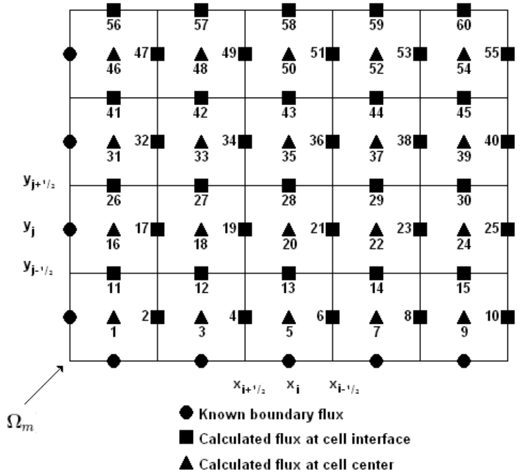
Main results

- Unified “analytical” solutions
- Concise, accurate, fast
- Mixtures: parameter analysis

Multidimensional Problems

- RGD: initial results
- NE: codes: iterative procedures, negative fluxes (corrections)

Geometry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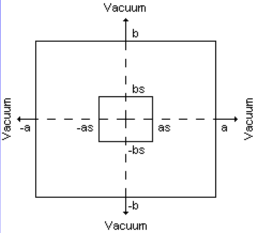
14
15
1
2
3
4
5
6
7
8
9
10
$y_{j+1/2}$
y_j
$y_{j-1/2}$
$x_{i+1/2}$
x_i
$x_{i-1/2}$
Ω_m
Known boundary flux
Calculated flux at cell interface
Calculated flux at cell center

Geometry



Nodal Schemes

- Closed Form Solutions
- Decoupled Problems (Lower order linear systems)
- Very Fast Solution
- No iterations

Tabela: Scalar flux $\phi(x)$, x=0.5

σ_s	Tsai & Loyalka N = 5, 7, 9, 11, 15	TWOTRAN-II N = 4, 8, 16	This work N = 2,4, 6, 8, 12, 16
	0.359604	0.337412	0.313
	0.358422	0.337707	0.335
0.50	0.357414	0.339794	0.337
	0.356678		0.338
	0.355885		0.340
			0.341
	0.258802	0.239483	0.221
	0.259150	0.241676	0.231
0.10	0.259131	0.244032	0.232
	0.259030		0.233
	0.258906		0.234
			0.235
	0.250097	0.231102	0.213
	0.250569	0.233421	0.222
0.05	0.250636	0.235787	0.223
	0.250591		0.224
	0.250529		0.225
			0.226

Concluding Comments

- Several Applications
  Computationally efficient codes

References

- L. B. Barichello and C. E. Siewert, A Discrete-Ordinates Solution for a Non-grey Model with Complete Frequency Redistribution, *JQSRT*, **62**, 665 (1999).
- C. S. Scherer, J. F. Prolo Filho and L. B. Barichello, An Analytical Approach to the Unified Solution of Kinetic Equations in the Rarefied Gas Dynamics. I. Flow Problems, *Z. Angew. Math. Phys.*, **60**, 70 (2009).
- C. S. Scherer, J. F. Prolo Filho and L. B. Barichello, An Analytical Approach to the Unified Solution of Kinetic Equations in the Rarefied Gas Dynamics. II. Heat-Transfer Problems, *Z. Angew. Math. Phys.*, **60**, 651 (2009).
- C. S. Scherer and L. B. Barichello, An analytical approach to the unified solution of kinetic equations in rarefied gas dynamics. III. Evaporation Problems, *Z. Angew. Math. Phys.*, 61, 95 (2010).
- Barichello, L. B., Cabrera, L. C., Prolo Filho, J. F., 2009. An Analytical Discrete Ordinates Solution for Two Dimensional Problems Based on Nodal Schemes. *2009 International Nuclear Atlantic Conference - INAC2009*, 27 Setembro – 02 de Outubro de 2009, Rio de Janeiro, RJ, Brasil. 10 p.

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